XSEDE High Performance Computing Use Cases

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A. Document History

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B. Document Scope

This document is both a user-facing document (publically accessible) and an internal working document intended to define user needs and use cases that fall under the general umbrella of High Performance Computing within the overall activities of XSEDE. The definition of use cases is based

on a template from Malan and Bredemeyer[1]. In general it is in keeping with the approaches and philosophy outlined in "Software architecture in practice."[2]

This document is one component of a process that generates at least the following documents, some of which are user-facing, some are as of now intended to be internal working documents:

- ***This document*** - A description of use cases [User facing]
- A binary mapping of use cases to Requirements in DOORS (a binary mapping – for each use case a "yes" or "no" flag indicating whether a particular requirement within the full list of requirements is or is not required to enable a particular use case).
- A set of level 3 decomposition documents, which include:
    - Quality Attributes descriptions
    - Connections diagram in UML

The use cases are presented here using the following format, derived from the Malan and Bredemeyer white paper[1] as follows:

Use Case	Use case identifier and reference number and modification history
Description	Goal to be achieved by use case and sources for requirement
References	References and citations relevant to use case
Actors	List of actors involved in use case
Prerequisites (Dependencies) & Assumptions	Conditions that must be true for use case to be possible Conditions that must be true for use case to terminate successfully
Steps	Interactions between actors and system that are necessary to achieve goal
Variations (optional)	Any variations in the steps of a use case
Quality Attributes	
Non-functional (optional)	List of non-functional requirements that the use case must meet
Issues	List of issues that remain to be resolved

[1] Malan, R., and D. Bredemeyer. 2001. Functional requirements and use cases. *www.bredemeyer.com/pdf_files/functreq.pdf*
[2] Bass, L., P Paul Clements, and Rick Kazman

C. Summary of Proposed HPC Use Cases

We define four XSEDE HPC Use cases, UCHPC1.0-4.0. What distinguishes these use cases from others is the need to obtain and sustain a high fraction of petascale floating point performance for every job.

UCHPC1.0: User (team) works with a single HPC system. For this use case, the following requirements are important:

- The user can learn quickly and correctly how to transfer files; build, run, debug, optimize, and run programs; and then sustain the pace of production that their project requires.
- The user is informed in a timely manner of any changes that will affect their pace of production, such as downtimes, software changes/updates (both general, e.g., O/S, compilers, MPI... and specific to the applications and libraries that they use), and policy changes (e.g., queue structure).
- The user is also able via an online mechanism to find out the status of their jobs, their SU account balance, etc.

UCHPC2.0: User (team) works with >1 HPC systems. For this use case, it is important that the conditions in use case 1 be fulfilled by all SPs in as consistent manner as is compatible with using each individual machine as efficiently as possible. E.g., it makes no sense to ask all SPs to run the same compiler or MPI library, but it makes sense to ask all SPs to use "modules", to provide consistent path names for libraries and 3rd party applications, to provide consistent end points for GridFTP / Globus Online, etc.

UCHPC3.0 User (team) runs an automated workflow engine. For this use case, it is important that the HPC system local environment(s) interface correctly with this workflow engine. This may require more stringent consistency among SPs than in UCHPC2.0, and also between HPC SPs and other SPs and non-XSEDE (e.g., campus bridged) resources the work and data flow may require. The workflow engine may be explicitly supported by the XSEDE architecture or it may require a new effort to make it work with the XSEDE architecture.

UCHPC4.0 User (team) needs customized changes to the HPC system(s). Such changes may include, for example, dedicated real-time processing of streaming data or a dedicated node to host a database.

D. Glossary

High Performance Computing (HPC): The means to solve the most numerically intensive problems that can be formulated at any given time, and that can be addressed with the computing technology available at that time. The technology available to XSEDE as of Q4, 2012 provides computers that achieve peak floating point performance in the N*F~ Petaflop/sec range, where

N~100,000 is the total number of processing units and F~10 Gigaflop/sec is the maximum possible performance of each processing unit.

HPC Service Provider (SP): An XSEDE SP whose Letter of Intent as accepted by XSEDE specifies the provision of an HPC System to the XSEDE community. The SP has staff members dedicated to the configuration and maintenance of an HPC System.

HPC System: Hardware, software, and operational policies deployed and maintained by an XSEDE SP for the purpose of satisfying the needs of HPC users. Examples of hardware: compute, login and I/O nodes, cores per node, accelerators, interconnects, storage systems, machine room and wide area networks. Examples of software: operating system, account management, compilers, libraries, debuggers, performance optimization tools, third-party HPC codes, batch queuing system, file transfer tools, data management tools. Examples of operational policies: definition of batch queues, rules regarding interactive access, maximum job execution time, maximum cores per job, job priorities, maximum number of concurrent jobs per user, storage quotas and retention times. It is the responsibility of the SP to configure and maintain the HPC system in accordance with their Cooperative Agreement with NSF and their SP Letter of Intent as accepted by XSEDE. *This configuration is expected to meet the needs of a well-defined set of HPC users.* We model each HPC system as a "box" with *interfaces* presented to its HPC users and XSEDE stakeholders. *The content of the HPC system "box" is dynamic, since many of its hardware, software and operational components change over the ~4 year time period that the system is provided to the XSEDE community. Changes in a HPC system may occur on timescales ranging from days to years.*

XSEDE Stakeholder: A member of the XSEDE Federation community, other than staff members at the SP that operates an HPC system, who needs to interact with this HPC system. Examples include members of the XSEDE AD&D, SD&I, Operations, TAS, TIS, User Support, ECSS and TEOS teams; also staff members at other SPs and on HPC user campuses.

HPC User: An XSEDE account holder focused on leading-edge compute-intensive problems whose solution requires applications that efficiently utilize the most capable XSEDE-allocated computers. HPC users can be single investigators or, more commonly, members of a research team in which they are assigned specific responsibilities in the HPC project.

HPC User Application: The set of codes and data employed by a HPC user. Codes and data can be developed, generated and maintained by HPC users, or by third parties. Even when third-party codes are used, the application data are unique to each HPC user group, since they are defined by their specific research problem. Data, including results from executing HPC User Jobs, may be stored on the HPC system, at the HPC User's home institution, at other XSEDE SPs or at other sites, for variable periods of time. They may be made available to a variety of stakeholders. The HPC User Application includes the mechanisms for data management and access, which are assumed to be compliant with the XSEDE User Responsibility Policy and the terms of the allocation under which the HPC User operates.

HPC User Job: An instance of a HPC User Application as executed on a HPC system. A job is specified by means of parameters defined by the HPC System, such as number of cores, execution time, and prerequisites (availability of input files, successful termination of a previous job, etc.)..

HPC User Job Performance: The number of scientifically significant results produced by each job in its specified execution time. In general, for HPC jobs, this number increases with the floating point rate the job sustains, i.e. with the number of cores it uses and the efficiency with which it uses them.

HPC User Project: The research program in support of which the XSEDE Allocations process has awarded an allocation to the HPC user. Each project has a budget of **"service units"** (SUs). Each job decrements the service unit balance by the product of the cores used and the run time.

HPC System Vendors: Third-party providers of components for a HPC System. It is part of the responsibilities of the HPC SP to interact with the vendors to ensure that the HPC system at all times meets the needs of its target set of HPC users.

Operational User Interface: The means for HPC users to work with an HPC system. This interface includes authenticating to the system; starting and ending interactive sessions; transferring data to and from the system; editing codes and data; building, debugging, and optimizing codes; launching and controlling jobs, and processing and managing their output. Interface components may be *local* or *remote* to the HPC system; they may be *manual* (each action requires direct intervention by the HPC user) or *programmatic* (multiple actions executed by a program launched by the HPC user).

Informational User Interface: The means for HPC users to learn the operational user interface of an HPC system, to learn about internal changes to the HPC system, and how these changes affect their use of the operational interface. It also provides HPC users with the means to report issues and give feedback to the SP. This interface includes documentation, training, user news, and user support. *This interface is not expected to be entirely automated. It is assumed that stakeholders provide its inputs and process its outputs.*

XSEDE Stakeholder Interface: The means for stakeholders to connect a HPC system to other resources coordinated or bridged by XSEDE. This interface includes the *remote* components of the system's operational user interface (e.g. file transfers, job scheduling and submission, data access and management from a system other than the HPC system); as well as synchronization of the HPC system with the XSEDE-wide allocation, accounting, authentication, resource discovery, documentation and user support systems. It provides stakeholders with the means to independently test the HPC system, to discover and report issues and give feedback to the SP.

XSEDE Common User Environment: Those elements of the Operational and Informational User Interfaces and of the Stakeholder Interface that are common to all XSEDE HPC systems. The TeraGrid project, as it passed the baton to XSEDE, has recommended the following common components of the *operational* interfaces of every HPC system: the CUE Management System -- an implementation of *Modules* on all systems, with 5 basic CUE modules and common module naming conventions for third-party applications; and the CUE Variable Collection, a set of common

environment variables to make resource discovery and job submission easier. They have also recommended a common standard for HPC system documentation (*informational user interface* implementation), including examples that show step by step how to build HPC user applications on each HPC system. For the *Stakeholder Interface*, they have recommended a CUE Testing Platform, a set of test programs that can be run to verify the functionality of the CUE components each SP is supposed to maintain. (The test programs can also be used as part of the *informational user interface*, illustrating the use of the CUE for the users.)

A. High Performance Computing Use Cases

UCHPC 1.0	User Project on a single HPC System
Description	An HPC User is assigned to execute a Project on a specific HPC System. The HPC SP and other relevant XSEDE stakeholders maintain the informational and operational user interfaces to the HPC system so that the User is in a position to complete all the project goals within the allocated time and SU budget. The project lifetime is one or more years.
References	TeraGrid Final Report, Section 3, 12/21/2011, http://hdl.handle.net/2142/43874 XD Service Providers Forum Charter : https://www.xsede.org/documents/10157/281380/SPF_Definition_v10.1_120228.pdf; specifically, Table 1.
Actors	• HPC User • HPC SP Staff and Vendors • XSEDE project stakeholders: Project office, operations, user services, extended collaborative support service (ECSS). • XSEDE federation stakeholders: Relevant staff at the HPC user's home institution, XD Technology Audit Service.
Prerequisites (Dependencies) and Assumptions	• The User, working within his or her research group, has formulated a Project to be completed within the time period and the SU budget allocated. • The user has prepared an initial version of the HPC Application that will be used to implement the Project. This work includes establishing the criteria for correctness of results, and the means to measure job performance.

	• The user knows the location of the Informational User Interface to the HPC System. • The user will only employ *manual* components of the Operational User Interface to the HPC System (no *programmatic* workflow engines will be employed). • The HPC Application does not include dynamic data sources (e.g. streaming from instruments); all necessary data reside on the HPC system for the duration of each Job. • The user will not utilize any SPs other than this HPC SP. • The user is assured of the cooperation of the staff members at his/her home institution, who are relevant to the execution of the Project (by configuring and maintaining the computing and communications infrastructure that will be used in conjunction with the HPC system).
Steps	• The User studies the Informational Interface to the HPC system to understand the Operational Interface. • The User transfers the Application to the HPC System, if not already present. • The User builds, tests, debugs and measures the performance of the Application on the HPC System. • The User decides which Application tasks (file transfers, jobs submission, output analysis and staging, data management) to perform *locally* on the HPC system, and which tasks (s)he will execute *remotely* (e.g. from the XSEDE User Portal, via a service such as Globus Online, or from her/his own workstation). • The User decides whether the Application requires any changes for correctness or better job performance ("optimization") on the HPC system. • The User optimizes the Application for the HPC system, until (s)he determines that all the Project goals can be completed within the allocated time and SU budget. • The User formulates a detailed sequence of Jobs to implement the Project. • The User begins executing the sequence of Jobs and reports any deviations from the expected behavior to XSEDE user services, who forward them to the HPC SP user support staff if necessary. • XSEDE stakeholders follow up as necessary in diagnosing user problem reports, including conducting tests of their own, forming "tiger teams" with the HPC SP staff, etc. • The User cooperates with all HPC SP and XSEDE stakeholder requests to follow up on problem reports, and to investigate specific issues related to the Application and the Jobs which execute it on the HPC system. • The User monitors the Informational Interface to the HPC System for any changes in the System that may require changes to the Application or to the Job sequence, including system down times and malfunctions. • The User manages the results of the Jobs, and other data relevant to the Project, using the mechanisms provided by the Application.

	• The User acknowledges XSEDE and the HPC SP in publications resulting from the Project, as required by the XSEDE User Responsibility Policy. The User cooperates with XSEDE stakeholder requests to generate reports, science stories, etc. based on the results of the Project.
Variations (optional)	The User requests the assistance of XSEDE ECSS staff in optimizing the Application for the HPC System.
Quality Attributes	• Time the user requires to achieve the first correct execution on the HPC system. ***At most 2 weeks after first login.*** • Time the user requires to obtain satisfactory job performance (to decide that the Project goals can be completed within the allocated time and SU budget). ***At most 4 weeks after first login.*** • Ratio of used to allocated service units by the end of the allocation period. ***At least 80%.*** • Does the user successfully apply for a follow-on XSEDE allocation? ***Yes.*** • Number of trouble tickets submitted by the user during the allocation period. ***Fewer than 10.*** • Distribution of resolution times for tickets submitted by the user during the allocation period. ***No resolution time greater than 1 week.*** • Positive statements made by the user regarding the contribution of the HPC system to the success of her/his Project, including the helpfulness of XSEDE and HPC SP staff in diagnosing and overcoming problems that have occurred during the execution of the Project. ***At least one quotable statement.*** • Number and quality (e.g. citations) of publications and scientific success stories resulting from the Project. ***At least one publication with at least 2 citations within 1 year of publication.***
Non-functional (optional)	ECS project progress reports, final report, and PI exit interview, if applicable.
Issues	• The "ideal" process outlined above assumes a high level of engagement and active cooperation between the User, HPC SP staff, and other XSEDE stakeholders. In practice, users are often slow to report problems, to seek assistance, and to act upon requests and recommendations by support staff. In turn, XSEDE and SP level processes are often still unable to inform the user of the causes of problems and the status of their remediation, within a time period the user perceives as satisfactory. • In particular, the "ideal" scenario outlined above assumes that the Allocations process has selected the projects that truly require the HPC system, by the user groups that are able to carry them out successfully i.e. that the prerequisites outlined above are most likely satisfied. In practice, the information conveyed to the reviewers e.g. about the performance of the user's application may be insufficient; overall

	constraints of allocating projects to XSEDE resources may result in suboptimal mappings of projects to HPC systems; etc. ● It is a challenge for staff at the SP level to easily communicate dynamic changes in their HPC system up to the XSEDE level. Some of the relevant changes can occur several times a week, sometimes unexpectedly, and neither existing automated processes nor staffing levels are adequate to reflect them for all users to become aware of in a timely manner. ● Training and documentation efforts at the XSEDE and SP levels need to become more proactive and targeted at teaching users how to best use each HPC system. ● Pertinent XSEDE architecture components such as EMS, XWFS and GFFS must be configured, tested, operated and maintained so that they work with the HPC systems at least as well as when a user ignores them and accesses each HPC system locally. ● Attention must be paid to the data management, storage, and analysis aspects of HPC projects. Petascale computations generate petascale data, and the XSEDE Federation should be prepared to facilitate adequate solutions to their management.

This is an information flow diagram representation of the Use Case (Use Case Diagram).

UCHPC 2.0	User Project on more than one HPC System
Description	An HPC User is assigned to execute a Project over an allocation period (e.g., one year) on multiple HPC Systems. The HPC SPs and other relevant XSEDE stakeholders maintain the informational and operational user interfaces to the HPC system so that the User is in a position to complete all the project goals within the allocated time and SU budget. For this, it is important that the conditions in use case 1 be fulfilled by all SPs in as consistent manner as is compatible with using each individual machine as efficiently as possible. E.g. it makes no sense to ask all SPs to run the same compiler or MPI library, but it makes sense to ask all SPs to use "modules", to provide consistent path names for libraries and 3rd party applications, to provide consistent end points for gridFTP / GlobusOnline, etc. **This is the XSEDE "Common User Environment" effort.**
References	TeraGrid Final Report, Section 3, 12/21/2011, http://hdl.handle.net/2142/43874 XD Service Providers Forum Charter : https://www.xsede.org/documents/10157/281380/SPF_Definition_v10.1_120228.pdf; specifically. Table 1. TeraGrid Common User Environment report: http://www.teragridforum.org/mediawiki/index.php?title=Dan_Summary_Requirements
Actors	• HPC User • Multiple HPC SP Staff and Vendors • XSEDE project stakeholders: Project office, operations, user services, extended collaborative support service (ECSS). • XSEDE federation stakeholders: Relevant staff at the HPC user's home institution, XD Technology Audit Service.
Prerequisites (Dependencies) and Assumptions	• The User, working within his or her research group, has formulated a Project to be completed within the time period and the SU budget allocated. • The user has prepared an initial version of the HPC Application(s) that will be used to implement the Project. This includes the criteria for correctness of results, and the means to measure job performance. • The user knows the location of the Informational User Interfaces to each

	of the HPC Systems allocated to the Project. XSEDE and the SPs must attempt to be as consistent as possible in location of the information and the content of the information (**"common user environment"**). ● The user will only employ *manual* components of the Operational User Interface to the HPC System (no *programmatic* workflow engines will be employed). ● The HPC Application(s) does not include dynamic data sources; all necessary data reside on the HPC systems for the duration of each Job. ● The user will utilize more than 1 SP. ● The user is assured of the cooperation of the staff members at his/her home institution, who are relevant to the execution of the Project (by configuring and maintaining the computing and communications infrastructure that will be used in conjunction with the HPC system).
Steps	● The User studies the Informational Interface to the HPC systems to understand the Operational Interfaces. ● The User transfers the Applications to the appropriate HPC Systems. ● The User builds, tests, debugs and measures the performance of the Applications on the HPC Systems. ● The User decides which Application tasks (file transfers, jobs submission, output analysis and staging, data management) to perform *locally* on each HPC system, and which tasks (s)he will execute *remotely* (e.g. from the XSEDE User Portal or from her/his own workstation). ● The User decides whether the Application requires any changes for correctness or better job performance ("optimization") on one or more of the HPC systems. ● The User optimizes the Application for the HPC systems, until (s)he determines that all the Project goals can be completed within the allocated time and SU budget. ● The User formulates a detailed sequence of Jobs to implement the Project. ● The User begins executing the sequence of Jobs and reports any deviations from the expected behavior to XSEDE user services, who forward them to the relevant HPC SP user support staff if necessary. ● The SPs are as consistent as possible considering compatibility with each individual machine. E.g. it makes no sense to ask all SPs to run the same compiler or MPI library, but it makes sense to ask all SPs to use "modules", to provide consistent path names for libraries and 3rd party applications, to provide consistent end points for GridFTP / Globus Online, etc. (**"common user environment"**). ● XSEDE stakeholders follow up as necessary in diagnosing user problem reports, including conducting tests of their own, forming "tiger teams" with the HPC SP staff, etc. ● The User cooperates with all HPC SP and XSEDE stakeholder requests to follow up on problem reports, and to investigate specific issues related to

	the Application and the Jobs that execute it on the HPC systems. ● The User monitors the Informational Interface to the HPC Systems for any changes in the System that may require changes to the Application or to the Job sequence, including system down times and malfunctions. ● The User manages the results of the Jobs, and other data relevant to the Project, using the mechanisms provided by the Application. ● The User acknowledges XSEDE and the HPC SPs in publications resulting from the Project, as required by the XSEDE User Responsibility Policy. The User cooperates with XSEDE stakeholder requests to generate reports, science stories, etc. based on the results of the Project.
Variations (optional)	The User requests the assistance of XSEDE ECSS staff in optimizing the Application for one or more of the HPC Systems.
Quality Attributes	● Time the user requires to achieve the first correct execution on all HPC systems. ***At most 4 weeks after first login.*** ● Time the user requires to obtain satisfactory job performance (to decide that the Project goals can be completed within the allocated time and SU budget). ***At most 8 weeks after first login.*** ● Ratio of performance sustained by the user's jobs to each HPC system's peak performance. ***At least 10%.*** ● Ratio of used to allocated service units by the end of the allocation period. ***At least 80%.*** ● Does the user successfully apply for a follow-on XSEDE allocation? ***Yes.*** ● Number of trouble tickets submitted by the user during the allocation period. ***Fewer than 15.*** ● Distribution of resolution times for tickets submitted by the user during the allocation period. ***No resolution time greater than 1 week.*** ● Positive statements made by the user regarding the contribution of the HPC systems to the success of her/his Project, including the helpfulness of XSEDE and HPC SP staff in diagnosing and overcoming problems that have occurred during the execution of the Project. ***At least one quotable statement.*** ● Number and quality (e.g. citations) of publications and scientific success stories resulting from the Project. ***At least one publication with at least 2 citations within 1 year of publication.***
Non-functional (optional)	ECS project progress reports, final report, and PI exit interview, if applicable.
Issues	● The "ideal" process outlined above assumes a high level of engagement and active cooperation between the User, HPC SP staff, and other XSEDE stakeholders. In practice, users are often slow to report problems, to seek assistance, and to act upon requests and recommendations by support staff. In turn, XSEDE and SP level processes are often still unable to inform

	the user of the causes of problems and the status of their remediation, within a time period the user perceives as satisfactory. • In particular, the "ideal" scenario outlined above assumes that the Allocations process has selected the projects that truly require the HPC systems, by the user groups that are able to carry them out successfully i.e. that the prerequisites outlined above are most likely satisfied. In practice, the information conveyed to the reviewers e.g. about the performance of the user's application may be insufficient; overall constraints of allocating projects to XSEDE resources may result in suboptimal mappings of projects to HPC systems; etc. • Is important that the conditions be fulfilled by all SPs in as consistent manner as is compatible with using each individual machine as efficiently as possible. **This is the XSEDE "Common User Environment" effort.** • It is a challenge for staff at the SP level to easily communicate dynamic changes in their HPC system up to the XSEDE level. Some of the relevant changes can occur several times a week, sometimes unexpectedly, and neither existing automated processes nor staffing levels are adequate to reflect them for all users to become aware of in a timely manner. • Training and documentation efforts at the XSEDE and SP levels need to become more proactive and targeted at teaching users how to best use each HPC system. • Pertinent XSEDE architecture components such as EMS, XWFS and GFFS must be configured, tested, operated and maintained so that they work with the HPC systems at least as well as when a user ignores them and accesses each HPC system locally. • Attention must be paid to the data management, storage, and analysis aspects of HPC projects. Petascale computations generate petascale data, and the XSEDE Federation should be prepared to facilitate adequate solutions to their management.

UCHPC 3.0	**Using a scientific workflow system to run on HPC systems**
Description	An HPC User is assigned to execute a Project on one or more HPC Systems, employing a **workflow system** to programmatically manage the HPC Application. The HPC SPs, workflow system providers and other relevant XSEDE stakeholders must maintain the informational and operational user interfaces of the HPC system(s), including programmatic interfaces to the workflow system, so that the User is in a position to complete all the project goals within the allocated time and SU budget.

References	**XSEDE Scientific Workflow Use Cases document** XD Service Providers Forum Charter : https://www.xsede.org/documents/10157/281380/SPF_Definition_v10.1_120228.pdf; specifically Table 1.
Actors	• HPC User • Support providers for the ***workflow system*** selected by the user • HPC SP Staff and their Vendors • XSEDE project stakeholders: Project office, operations, user services, extended collaborative support service (ECSS). • XSEDE federation stakeholders: Relevant staff at the HPC user's home institution, XD Technology Audit Service.
Prerequisites (Dependencies) and Assumptions	• The User, working within his or her research group, has formulated a Project to be completed within the time period and the SU budget allocated. • The user has prepared an initial version of the HPC Application(s) that will be used to implement the Project. This includes the criteria for correctness of results, and the means to measure job performance. • The user knows the location of the Informational User Interfaces to each of the HPC Systems allocated to the Project. XSEDE and the SPs must attempt to be as consistent as possible in location of the information and the content of the information (**"common user environment"**). • The user has selected a ***workflow system*** to interact ***programmatically*** with the Operational User Interfaces to the HPC System(s). • The user is assured of the cooperation of the staff members at his/her home institution, who are relevant to the execution of the Project (by configuring and maintaining the computing and communications infrastructure that will be used in conjunction with the HPC system). • The user is assured of the cooperation of the support providers for the selected ***workflow system.*** These may include staff at his/her home institution, third-party providers, and XSEDE Project Stakeholders.
Steps	• The User studies the Informational Interface to the HPC systems to understand the Operational Interfaces. • The User selects a Workflow System that will interact programmatically with the Operational and Informational Interfaces. • The User transfers the Application (including the relevant components of the Workflow System) to the HPC Systems. • The User decides how best to use the Workflow System to programmatically launch and manage HPC Jobs on the HPC Systems. • The User configures the Workflow System accordingly. • The User builds, tests, debugs and measures the performance of the Application on the HPC Systems. **This includes the ratio of the number of scientifically**

	significant results produced per unit time with and without the Workflow System. ● The User decides whether the Application (including the Workflow System) requires any changes for correctness or better job performance ("optimization") on one or more of the HPC systems. ● The User optimizes the Application (including the relevant configuration or features of the Workflow System) for the HPC systems, until (s)he determines that all the Project goals can be completed within the allocated time and SU budget. ● The User formulates a detailed sequence of Jobs to implement the Project. ● The User begins executing the sequence of Jobs and reports any deviations from the expected behavior to XSEDE user services, who forward them to the relevant HPC SP user support staff if necessary. ● If the User has evidence, from the Workflow System's monitoring component, that the Workflow System deviates from its expected behavior, (s)he includes this information in the report to XSEDE user services, as well as to the Support Providers for the Workflow System (if these are external to XSEDE). ● XSEDE stakeholders follow up as necessary in diagnosing user problem reports, including conducting tests of their own, forming "tiger teams" with the Support Providers for the Workflow System, HPC SP staff, etc. ● The User cooperates with all HPC SP, XSEDE stakeholder and Workflow System provider requests to follow up on problem reports, and to investigate specific issues related to the Application and the Jobs that execute it on the HPC systems. ● The User monitors the Informational Interface to the HPC Systems for any changes in the System that may require changes to the Application (including the configuration of the Workflow System) or to the Job sequence, including system down times and malfunctions. ● The User manages the results of the Jobs, and other data relevant to the Project, using the mechanisms provided by the Application. ● The User acknowledges XSEDE and the HPC SPs in publications resulting from the Project, as required by the XSEDE User Responsibility Policy. The User cooperates with XSEDE stakeholder requests to generate reports, science stories, etc. based on the results of the Project. In particular, use of an XSEDE supported Workflow System should be acknowledged. ● The User will also want to acknowledge any non-XSEDE Workflow System Provider in the resulting publications.
Variations (optional)	The User requests the assistance of XSEDE ECSS staff in optimizing the Application (including the Workflow System if necessary).
Quality Attributes	● Time the user requires to achieve the first correct execution of the complete Application on the set of all HPC systems, by means of the Workflow System. ***At most 6 weeks after work begins.*** ● Time the user requires to obtain satisfactory job performance (to decide that the Project goals can be completed within the allocated time and SU budget).

	At most 10 weeks after work begins. ● Ratio of the scientifically significant results obtained per unit time, with and without using the Workflow System. ***At least 1.25.*** ● Ratio of performance sustained by the user's jobs to each HPC system's peak performance. ***At least 10%.*** ● Ratio of used to allocated service units by the end of the allocation period. ***At least 80%.*** ● Does the user successfully apply for a follow-on XSEDE allocation? ***Yes.*** ● Number of trouble tickets submitted by the user during the allocation period. ***Fewer than 25.*** ● Distribution of resolution times for tickets submitted by the user during the allocation period. ***No resolution time greater than 2 weeks.*** ● Positive statements made by the user regarding the contribution of the HPC system to the success of her/his Project, including the helpfulness of XSEDE and HPC SP staff in diagnosing and overcoming problems that have occurred during the execution of the Project. ***At least one quotable statement.*** ● Number and quality (e.g. citations) of publications and scientific success stories resulting from the Project. ***At least one publication with at least 2 citations within 1 year of publication.***
Non-functional (optional)	ECS project progress reports, final report, and exit interview, if applicable.
Issues	● As discussed in the Scientific Workflows Use Cases document, the user may bring their own workflow system as part of their application (just as they can bring their own HPC codes), or they may opt to use a workflow system supported (in whole or in part) by XSEDE. ● In any case, the support and possibly the development personnel of the workflow system provider will be added to the list of actors, resulting in more complex problem solving interactions than for HPC use cases 1 and 2. ● The goal remains to utilize each HPC system efficiently. The additional overhead of setting up and operating the workflow system should be more than offset by the productivity gain, measured in scientifically significant results obtained per unit time. ● As of May 2013, few HPC user teams are familiar with Workflow Systems and their benefits. XSEDE ECSS is engaging in a proactive effort to increase awareness and expertise, but until this bears fruit, the above goal will be difficult to achieve. ● Specifically, if the user's application requires coding changes in the workflow system to meet the project goals, use of the workflow system may have to be postponed until the next allocation year. ● The "ideal" process outlined above assumes a high level of engagement and active cooperation between the User, HPC SP staff, workflow system providers, and other XSEDE stakeholders. ● In particular, the "ideal" scenario outlined above assumes that the Allocations process has selected the projects that truly require the workflow system

	proposed, by the user groups that are able to carry them out successfully i.e. that the prerequisites outlined above are most likely satisfied. In practice, the information conveyed to the reviewers e.g. about the performance of the user's application may be insufficient; overall constraints of allocating projects to XSEDE resources may result in suboptimal mappings of projects to HPC systems; etc. Most reviewers are not yet familiar with workflow systems, so until they are, they cannot be expected to help with the selection of a suitable system. ● Is important that the conditions be fulfilled by all SPs in as consistent manner as is compatible with using each individual machine as efficiently as possible. ● It is a challenge for staff at the SP level to easily communicate dynamic changes in their HPC system up to the XSEDE level. Some of the relevant changes can occur several times a week, sometimes unexpectedly, and neither existing automated processes nor staffing levels are adequate to reflect them for all users to become aware of in a timely manner. ● Most SP staff are not yet familiar with workflow systems, so until they are, they may require considerable help from the workflow system providers and XSEDE stakeholders. ● It is also likely that some of the dynamic changes in the HPC systems will negatively impact the correct functioning and/or the performance of the workflow system. Complex and lengthy interactions between the SP staff and the other actors may be required to diagnose and fix these problems. In some cases, the SP will have to undo the changes. ● Training and documentation efforts at the XSEDE and SP levels need to become more proactive and targeted at teaching users how to best use each HPC system. An aggressive and efficient program to teach users, XSEDE and SP staff about Workflow Systems is essential for this use case to become widely and successfully adopted.